Comment on "Aging Effects in a Lennard-Jones Glass"

In a recent Letter Kob and Barrat[1] reported results of molecular dynamics simulations for the off-equilibrium dynamics in a binary Lennard-Jones (LJ) glass. The main conclusions of their work was 1) they find aging in this glassy systems and 2) that they find a *simple* aging scenario close to a t/t_w scaling, which is very reminiscent of comparable studies in spin glasses. In this comment we would like to emphasize that a different aging scenario, known under the name *activated dynamics* scaling, is much more appropriate for the system under consideration than the one proposed by Kob and Barrat[1].

For this reason we repeated the simulation by Kob and Barrat, using exactly the same potential (Lennard-Jones for a binary mixture), the same parameters (same diameters, mixture, density and temperatures) and the same quenching procedure (T_i=5, T_f=0.4) however with much larger systems ($32768 = 32^3$ particles) and similar times ($2 \cdot 10^6$ time steps, 1 time step corresponding to 0.01 LJ-units). The aging properties of the system manifest themselves in the two-time autocorrelation function

$$C_q(t+t_w,t_w) = \frac{1}{N}\sum_i e^{i\cdot q\cdot[r_i(t+t_w)-r_i(t_w)]} \;, \qquad (1)$$

where $r_i(t)$ is the position of particle i at time t and the absolute value of q corresponds to the first maximum in the structure function. We choose 100 randomly distributed vectors and averaged C_q over these vectors. The function (1) was evaluated after every 10 time steps and 5^n measurements were averaged over to improve statistics. We convinced ourselves that different quenching procedures with identical initial and final temperatures, T_i and T_f, lead to the same scaling behavior.

In [1] it has been suggested that $C_q(t+t_w,t_w)$ obeys

$$C_q(t+t_w,t_w) \sim \tilde{c}(t/t_r) \qquad (2)$$

with a relaxation time $t_r \propto t_w^\alpha$. We checked this *Ansatz* for our data and display the result in the inset of Fig. 1, surprisingly we find an exponent $\alpha \sim 1.1$, very close to one (corresponding to simple t/t_w scaling) but different from the one $\alpha = 0.88$ reported in [1]. The data collapse in the asymptotic regime is not at all satisfying, the data for different waiting times conincide exactly only for $C_q = 0.45$. For this reason we tried another aging scenario, proposed in the context of spin glasses by Fisher and Huse[2], which we call the *activated dynamics*:

$$C_q(t+t_w,t_w) \sim \tilde{C}\{\ln((t+t_w)/\tau)/\ln(t_w/\tau)\} \qquad (3)$$

where τ is a fit-parameter and plays the role of an effective microscopic time scale. Fig.1 we show the scaling plot for such a scenario, which gives a much better data collapse in the asymptotic regime $t \geq t_w$.

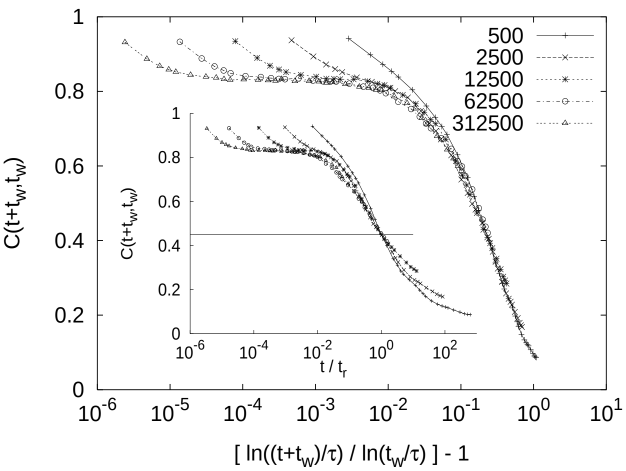

FIG. 1. Activated dynamics scaling plot according to eq.(3) with $\tau = 0.5$. Note that we shifted the scaling variable by 1 to the left to have a better resolution of the crossover region. The inset shows a scaling plot of our data according to the scenario proposed by Kob and Barrat [1], see eq.(2), the full line corresponds to $C_q = 0.45$. The relaxation times are t_r=1450, 10600, 70000, 600000 and 3000000 for t_w=500, 2500, 12500, 62500 and 312500, roughly a dependence $t_r \propto t_w^{1.1}$.

The origin of such an activated dynamics scaling in spin glass phenomenology[2] is simply a logarithmically slow coarsening process $\xi(t) \sim \ln(t)^a$, where $\xi(t)$ is a time dependent spatial correlation length and a some exponent. This plus the observation that in coarsening dynamics the two time correlation function $C_q(t+t_w,t_w)$ should depend on the ration of the two length scale $\xi(t_w)/\xi(t+t_w)$ alone yields the aging behavior (3).

Three things are worth being noted: 1) In the context, in which (3) was first suggested, namely the 3d EA spin glass, this form does not seem to work[3]. 2) Only very recently a growing length scale has been observed in the very same model we are considering here[4]. 3) An even better data collapse can be obtained by plotting $C_q(t+t_w,t_w)$ versus $\ln(t)/\ln(t_r)$, with a relaxation time t_r individually chosen for each waiting time t_w. Here it turns out that $t_r(t_w)$ grows faster than with a power law.

To conclude we have shown that the aging behavior of a Lennard-Jones glass is more appropriately described by an activated dynamics scaling rather than simple aging, as claimed by Kob and Barrat in [1].

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